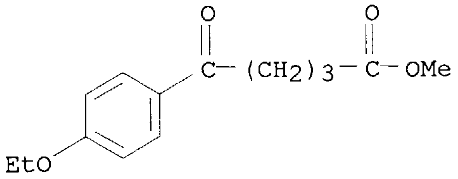
(Reactant or reagent)
(preparation and Grignard reaction of, in bis(alkoxyphenyl)ethylenecarboxylates manufacture)

RN 152629-77-1 CAPLUS

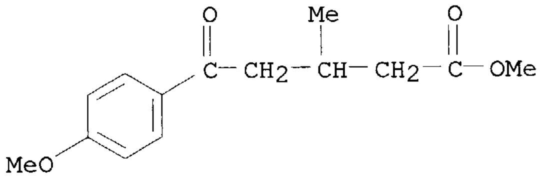
CN Benzenepentanoic acid, 4-ethoxy-δ-oxo-, methyl ester (9CI) (CA INDEX NAME)



RN 152629-78-2 CAPLUS

CN Benzenepentanoic acid, 4-methoxy-β-methyl-δ-oxo-, methyl ester (9CI) (CA INDEX NAME)

INT 660



AB The title derivs. (R1O-p-C6H4)2C:CR2(ACO2R3) [R1 = lower alkyl; R2 = halo; R3 = H, lower alkyl; A = (lower alkyl-substituted) C1-4 alkylene], and their **pharmaceutically acceptable salts** are prepared as platelet aggregation inhibitors, antithrombotics, and antiphlogistics (no data). Refluxing a mixture of 2.61 g Me 5,5-bis(4-methoxyphenyl)-4-pentenoate [prepared from Me 4-(4-methoxybenzoyl)butyrate in 2 steps] and 1.60 g N-chlorosuccinimide in CH2Cl2 for 10 h gave 2.50 g Me 4-chloro-5,5-bis(4-methoxyphenyl)-4-pentenoate.

L12 ANSWER 77 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1993:649709 CAPLUS
DN 119:249709
TI Sulfamates as antiglaucoma agents
IN Lo, Young S.; Nolan, Joseph C.; Shamblee, Dwight A.
PA A. H. Robins Co., Inc., USA
SO U.S., 35 pp. Cont-in-part of U.S. Ser. No. 406,736, abandoned.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 1

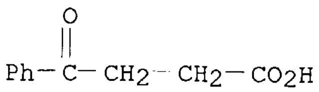
| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|---|
| PI | US 5192785 | A | 19930309 | US 1991-712855 | 19910610 |
| | | | | US 1989-406736 | 19890903 |

OS MARPAT 119:249709
IT **2051-95-8**, 3-Benzoylpropionic acid
RL: RCT (Reactant); RACT (Reactant or reagent)

(borane reduction of, diol from)

RN 2051-95-8 CAPLUS

CN Benzenebutanoic acid, γ-oxo- (9CI) (CA INDEX NAME)



$Ph-\overset{\overset{O}{||}}{C}-CH_2-CH_2-CO_2H$

AB Sulfamates (HO)pA[OS(O)2NR1R2]z (A = aryloxyalkyl, p = number of OH groups present on the alkyl moiety of A which have not been converted to OS(O)2NR1R2 groups, including 0; z = number of OS(O)2NR1R2 groups attached to carbons of the alkyl moiety and is ≥ 1; R1 and R2 are selected from H, lower alkyl, carboxy, etc.] are prepared by three methods: (1) condensation of an alc. with a chlorosulfamate at low temperature, (2) reaction of an aryl sulfamate and alc. at higher temps., or (3) by condensation of an aryl alc. with chlorosulfonyl isocyanate at 80-150° in a non-reactive aprotic solvent with subsequent hydrolysis and CO2 elimination. The sulfamates and their **pharmaceutically acceptable salts** and formulations are useful for reducing intraocular pressure in mammals. Examples include 137 syntheses, 42 precursor prepns., and intraocular pressure results for 5 compds. in rabbits.

L12 ANSWER 78 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1993:625694 CAPLUS

DN 119:225694

TI Preparation of bis(4-alkoxyphenyl)alkenoate derivatives as platelet aggregation inhibitors, antiinflammatories, and analgesics

IN Ito, Yasuo; Kato, Hideo; Yasuda, Shingo; Ogawa, Nobuo; Suzuki, Tomio; Sakurai, Shunichiro

PA Hokuriku Pharmaceutical, Japan

SO Jpn. Kokai Tokkyo Koho, 5 pp.
CODEN: JKXXAF

DT Patent

LA Japanese

FAN.CNT 1

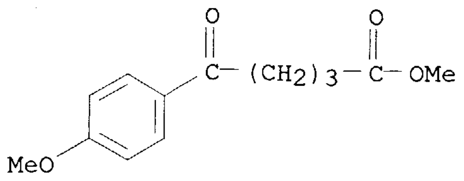
| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|---|
| PI | JP 05170696 | A2 | 19930709 | JP 1991-354510 | 19911220 |
| | | | | JP 1991-354510 | 19911220 |

OS MARPAT 119:225694

IT **1847-68-3**
RL: RCT (Reactant); RACT (Reactant or reagent)
(Grignard reaction of, with bromoanisole)

RN 1847-68-3 CAPLUS

CN Benzenepentanoic acid, 4-methoxy-δ-oxo-, methyl ester (9CI) (CA INDEX NAME)



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 NEWS  3  SEP 09   CA/CAplus records now contain indexing from 1907 to the
                   present
 NEWS  4  DEC 08   INPADOC: Legal Status data reloaded
 NEWS  5  SEP 29   DISSABS now available on STN
 NEWS  6  OCT 10   PCTFULL: Two new display fields added
 NEWS  7  OCT 21   BIOSIS file reloaded and enhanced
 NEWS  8  OCT 28   BIOSIS file segment of TOXCENTER reloaded and enhanced
 NEWS  9  NOV 24   MSDS-CCOHS file reloaded
 NEWS 10  DEC 08   CABA reloaded with left truncation
 NEWS 11  DEC 08   IMS file names changed
 NEWS 12  DEC 09   Experimental property data collected by CAS now available
                   in REGISTRY
 NEWS 13  DEC 09   STN Entry Date available for display in REGISTRY and CA/CAplus
 NEWS 14  DEC 17   DGENE: Two new display fields added
 NEWS 15  DEC 18   BIOTECHNO no longer updated
 NEWS 16  DEC 19   CROPU no longer updated; subscriber discount no longer
                   available
 NEWS 17  DEC 22   Additional INPI reactions and pre-1907 documents added to CAS
                   databases
 NEWS 18  DEC 22   IFIPAT/IFIUDB/IFICDB reloaded with new data and search fields
 NEWS 19  DEC 22   ABI-INFORM now available on STN
 NEWS 20  JAN 27   Source of Registration (SR) information in REGISTRY updated
                   and searchable
 NEWS 21  JAN 27   A new search aid, the Company Name Thesaurus, available in
                   CA/CAplus
 NEWS 22  FEB 05   German (DE) application and patent publication number format
                   changes
 NEWS 23  MAR 03   MEDLINE and LMEDLINE reloaded
 NEWS 24  MAR 03   MEDLINE file segment of TOXCENTER reloaded
 NEWS 25  MAR 03   FRANCEPAT now available on STN

 NEWS EXPRESS  MARCH 5 CURRENT WINDOWS VERSION IS V7.00A, CURRENT
               MACINTOSH VERSION IS V6.0b(ENG) AND V6.0Jb(JP),
               AND CURRENT DISCOVER FILE IS DATED 3 MARCH 2004
 NEWS HOURS    STN Operating Hours Plus Help Desk Availability
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=> file reg
COST IN U.S. DOLLARS                               SINCE FILE      TOTAL
                                                        ENTRY    SESSION
FULL ESTIMATED COST                                      0.21       0.21

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DICTIONARY FILE UPDATES:   16 MAR 2004  HIGHEST RN 663883-43-0

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

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  conducting SmartSELECT searches.

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Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

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Uploading c:\program files\stnexp\queries\10684730.1

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L1              STR
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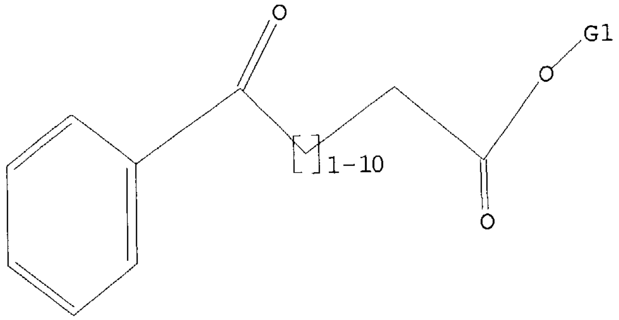

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G1 H,Ak



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FULL SCREEN SEARCH COMPLETED -  87741 TO ITERATE

100.0% PROCESSED   87741 ITERATIONS                        12500 ANSWERS
SEARCH TIME: 00.00.03

L2         12500 SEA SSS FUL L1

=> file caplus
COST IN U.S. DOLLARS                               SINCE FILE      TOTAL
                                                        ENTRY    SESSION
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FILE LAST UPDATED: 16 Mar 2004  (20040316/ED)

  This file contains CAS Registry Numbers for easy and accurate
  substance identification.


=> s l2
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L3         8378 L2

=> s l3 and difluoro
L4           54 L3 AND DIFLUORO

=> d l4 fbib hitstr abs total

L4   ANSWER 1 OF 54  CAPLUS  COPYRIGHT 2004 ACS on STN
AN   2004:41443  CAPLUS
DN   140:93936
TI   Preparation of secondary amino anilinic piperidines as selective MCH1
     antagonists with therapeutic uses
IN   Marzabadi, Mohammad; Jiang, Allen; Lu, Kai; Chen, Chien-An; Deleon, John;
     Wetzel, John
PA   Synaptic Pharmaceutical Corporations, USA
SO   PCT Int. Appl., 129 pp.
     CODEN: PIXXD2
DT   Patent
LA   English
FAN.CNT 1
     PATENT NO.        KIND  DATE          APPLICATION NO.  DATE
     ---------------   ----  --------      ---------------  --------
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             CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
             GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
             LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM,
             PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN,
             TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY,
             KG, KZ, MD, RU
        RW:  GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG,
             CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC,
             NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ,
             GW, ML, MR, NE, SN, TD, TG
                                               US 2002-189145 A220020703
OS   MARPAT 140:93936
IT   4144-62-1, 6-Oxo-6-phenylhexanoic acid
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (preparation of secondary amino anilinic piperidines as selective MCH1
        antagonists with therapeutic uses)
RN   4144-62-1  CAPLUS
CN   Benzenehexanoic acid, ε-oxo- (9CI)  (CA INDEX NAME)
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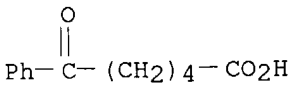

$Ph-\overset{O}{\overset{\|}{C}}-(CH_2)_4-CO_2H$

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GI
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GI

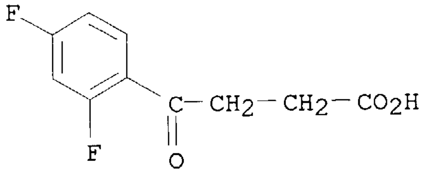
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The title compds. I [R1, R2 = H, hydroxy, (subsitituted) alkyl, etc.; R3 = alkyl; R4 = H, (protected) amino, etc.; Z = O, S, etc.; m, n = 0 - 2] are prepared Title compound II HCl **salt** (R1 = R2 = H) (preparation given) was isolated as isomer A , [α]D = +178°, and isomer B, [α]D = -38°. Said isomer A in vitro showed IC50 of 3.38 ng/mL against P388 mouse leukemic cells. Said isomer B in vitro showed IC50 of 12.40 ng/mL against P388 mouse leukemic cells. Title compound II HCl **salt** (R1 = Me; R2 = F) in vitro showed IC50 of 0.58 ng/mL against P388 mouse leukemic cells. Title compound II HCl **salt** (R1 = Me; R2 = F) at 12.5 mg/Kg i. v. gave 56.5% inhibition of tumor in mice with transplanted Meth A tumor.

L13 ANSWER 8 OF 8 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1989:423238 CAPLUS
DN 111:23238
TI New allylamine derivatives, their preparation, and their use as antimycotics
IN Nussbaumer, Peter; Stuetz, Anton; Vyplel, Hermann; Enzersdorf, Maria
PA Sandoz-Patent-G.m.b.H., Fed. Rep. Ger.
SO Ger. Offen., 10 pp.
CODEN: GWXXBX
DT Patent
LA German
FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|---|
| PI | DE 3720317 | A1 | 19881229 | DE 1987-3720317<br>DE 1987-3720317 | 19870619<br>19870619 |

OS CASREACT 111:23238; MARPAT 111:23238
IT **110931-77-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, in synthesis of allylnaphthylmethylamine fungicide)
RN 110931-77-6 CAPLUS
CN Benzenebutanoic acid, 2,4-difluoro-γ-oxo- (9CI) (CA INDEX NAME)



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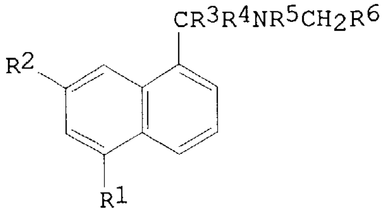

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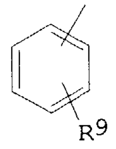

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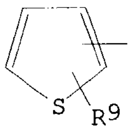

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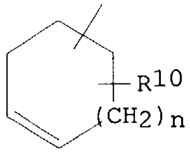

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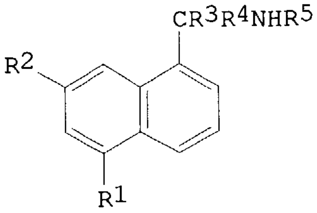
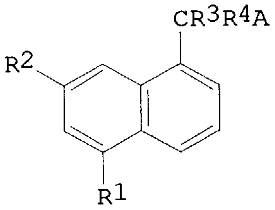


II



III

AB Naphthalenes I [R1,R2 = H, F; R1 = R2 ≠ H; R3, R4, R5 = H, alkyl; R4, R5 = (CH)2)m ; R5 = CH:CHC.tplbond.CR7, CH:CHCH:CHR7, CH2C.tplbond.CR78 CH:CHR8; R7 = alkyl, cycloalkyl, trialkylsilyl, dialkylphenylsilyl, phenylalkyl, or alkenyl (un)substituted by alkyl, alkoxy, Ph, or halo; R8 = Q, Q1, Q2; R9 = halo, CF3, alkyl, alkyl, H; R10 = H, alkyl; m = 3,4,5; n = 0-2] and their acid **salts**, useful as medicinal and agrochem. fungicides, were prepared:a) by reaction of amine II with ACH2R6 (A = cleavable group), or b) by reaction of III with R5NH = CH2R6 and optional conversion of the products into acid addition **salts**. Me3CC.tplbond.CCH:CHCH2Br [(E):(Z) = 3:1] in DMF was added dropwise to (5,7-difluoro-1-naphthylmethyl)methylamine (prepared in 7 steps from 1,3-F2C6H4, AlCl3, and succinic anhydride) and K2CO3 in DMF and the mixture kept 4 h at room temperature to give (E)- and (Z)-I (R1 = R2 = F, R3 =
R4
= H, R5 = Me, R6 = CH:CHC.tplbond.CCMe3) (V). The curative dose for V in treating guinea pigs infected with Trichophyton mentagrophytes was 9 + 6 mg/kg in miglyol vs. 9 + 70 mg/kg for griseofulvin.

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=> d l15 fbib hitstr abs total
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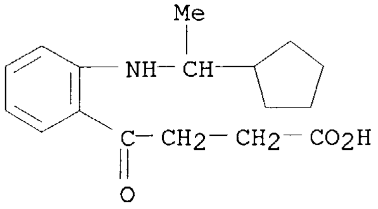
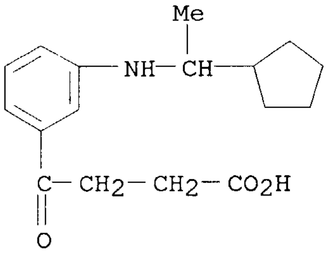
L15 ANSWER 1 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2004:41443 CAPLUS
DN 140:93936
TI Preparation of secondary amino anilinic piperidines as selective MCH1 antagonists with therapeutic uses
IN Marzabadi, Mohammad; Jiang, Allen; Lu, Kai; Chen, Chien-An; Deleon, John; Wetzel, John
PA Synaptic Pharmaceutical Corporations, USA

CN Benzenebutanoic acid, 2-[(1-cyclopentylethyl)amino]-γ-oxo- (9CI) (CA INDEX NAME)



RN 80230-54-2 CAPLUS
CN Benzenebutanoic acid, 3-[(1-cyclopentylethyl)amino]-γ-oxo- (9CI) (CA INDEX NAME)



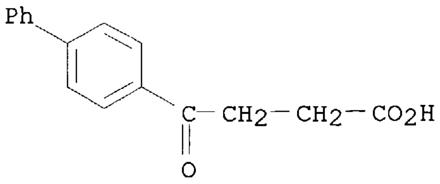
AB The title compds. 2- and 3-RC6H4NR1ZnR2 [I; R = carbonyl-, carboxy-, amido-, or iminooxyalkyl-containing moiety; R1 = H or group convertible in vivo thereto; Z = C1-13 alkylene or alkenylene optionally substituted (o.s.) with ≥1 C1-4 alkyl; n = 0, 1; R2 = C3-16 cycloalkyl or C4-17 cycloalkenyl o.s. by ≥1 C1-13 alkyl, C4-8 cycloalkyl, decahydronaphthyl, :CH2, :CHMe, :CMe2; the total number of C atoms in Z and R2 ≤20] and their **pharmaceutically acceptable salts** are described. I are useful as hypolipidemic and antiatherosclerotic agents (no data). E.g., 2-(2-cyclopentylethylamino)phenylacetic acid was prepared from 2-cyclopentylethanol by sequential methylsulfonylation, treatment with 2-H2NC6H4CH2CO2Et (HMPT, 120°, 20 h), and hydrolysis.

L12 ANSWER 99 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1976:483243 CAPLUS
DN 85:83243
TI 3-(4-Biphenylcarbonyl)propionic acid as an inhibitor of platelet aggregation
IN Ellenbogen, Leon; Kohler, Constance A.
PA American Cyanamid Co., USA
SO U.S., 4 pp.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|---|
| PI | US 3966960 | A | 19760629 | US 1975-571826 | 19750425 |

US 1975-571826 19750425

IT **36330-85-5**
RL: BIOL (Biological study)
(in pharmaceuticals, for blood platelet aggregation inhibition)
RN 36330-85-5 CAPLUS
CN [1,1'-Biphenyl]-4-butanoic acid, γ-oxo- (9CI) (CA INDEX NAME)



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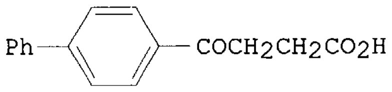

I

AB The use of 3-(4-biphenylcarbonyl)propionic acid (I) [**36330-85-5**] and its **pharmaceutically acceptable salts** to inhibit blood platelet aggression and thrombosis formation and compns. containing such compds. were reported. The synthesis of I was also reported. Thus, to 135 g AlCl3 dissolved in 500 ml nitrobenzene at <10° was added 50 g succinic anhydride [108-30-5] and 75 g biphenyl [92-52-4] with stirring and temperature retention <10°. The reaction mixture was poured into 150 ml concentrated HCl in 1l. ice water, the nitrobenzene removed by steam distillation, the solid collected, dissolved in 4 l. 3% Na2CO3, clarified, and repptd. with excess 6N H2SO4 to give I, m.p. 185-7°. I 10.0, Mg stearate 0.2, and lactose 12.0 g were placed in 100 gelatin capsules.

L12 ANSWER 100 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1972:535298 CAPLUS
DN 77:135298
TI Prophylaxis and treatment of cardiac disorders with benzoyl compounds
IN Garzia, Aldo
PA Istituto Chemioterapico Italiano S.p.A.
SO S. African, 15 pp.
CODEN: SFXXAB
DT Patent
LA English
FAN.CNT 2

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|---|
| PI | ZA 7104112 | A | 19720329 | ZA 1971-4112 | 19710623 |
| | | | | US 1970-50325 | 19700626 |
| | US 3803222 | A | 19740409 | US 1970-50325 | 19700626 |
| | GB 1323008 | A | 19730711 | GB 1971-17692 | 19710527 |
| | | | | US 1970-50325 | 19700626 |
| | BE 768809 | A1 | 19711103 | BE 1971-104881 | 19710621 |

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     FR 2100826          A5    19720324
                                                  US 1970-50325     19700626
     US 3857949          A     19741231           US 1972-226985    19720216
                                                  US 1970-50325     19700626
PATENT FAMILY INFORMATION:
FAN  1972:149219
     PATENT NO.          KIND  DATE               APPLICATION NO.   DATE
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PI   DE 2131676          A     19720127           DE 1971-2131676   19710625
                                                  US 1970-50325     19700626
     US 3803222          A     19740409           US 1970-50325     19700626
     GB 1323008          A     19730711           GB 1971-17692     19710527
                                                  US 1970-50325     19700626
     BE 768809           A1    19711103           BE 1971-104881    19710621
                                                  US 1970-50325     19700626
     FR 2100826          A1    19720324           FR 1971-23115     19710624
     FR 2100826          A5    19720324
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     US 3857949          A     19741231           US 1972-226985    19720216
                                                  US 1970-50325     19700626
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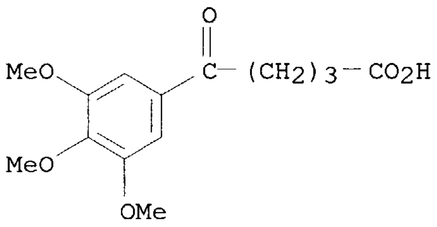
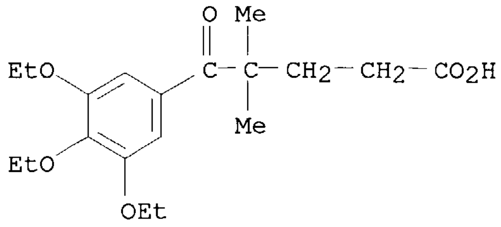
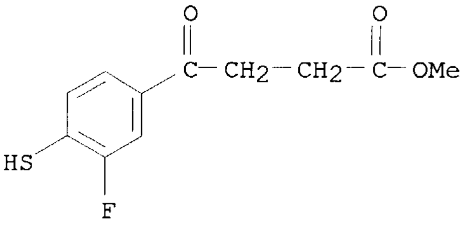
IT **34759-04-1**
RL: BIOL (Biological study)
(in heart disease prevention and treatment)
RN 34759-04-1 CAPLUS
CN Benzenepentanoic acid, 3,4,5-trimethoxy-δ-oxo- (9CI) (CA INDEX NAME)



IT **36708-50-6P 36708-51-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 36708-50-6 CAPLUS
CN Benzenepentanoic acid, 3,4,5-triethoxy-γ,γ-dimethyl-δ-oxo- (9CI) (CA INDEX NAME)





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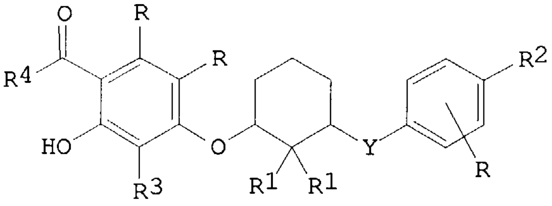

I

INT

AB Title compds. I [Y = O, S, SO, SO2; R = H, C1-6 alkyl, CF3, halo, (alkyl)amino; R1 = H, C1-6 alkyl, OH, alkoxy; R2 = R5CqR6R7CrR6R7 Cp(O); p = 0, 1; q, r = 0-3; R5 = CO2R1; R6 = H, C1-4 alkyl; R7 = H, OH, C1-4 alkyl; R3 = C1-6 alkyl, alkenyl; R4 = C1-6 alkyl] and their **pharmaceutically acceptable salts** are prepared as leukotriene antagonists (no data). A mixture of 0.72 g trans-3-(4-acetyl-3-hydroxy-2-propylphenoxy)-1,2-epoxidocyclohexane and 0.91 g Me 4-mercaptobenzeneacetate was refluxed for 2 days in MeOH in the presence of Et3N to give a (carbomethoxymethylphenylthio)cyclohexane which was base hydrolyzed to give trans,trans-3-(4-acetyl-3-hydroxy-2-propylphenoxy)-2-hydroxy-1-(4-carboxymethylphenylthio)cyclohexane.

L12 ANSWER 93 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1988:186735 CAPLUS
DN 108:186735
TI Preparation of 3-substituted 1,5-diphenylpyrazoles as antiinflammatories
IN Wachter, Michael Paul; Ferro, Michael Paul
PA Ortho Pharmaceutical Corp., USA
SO Eur. Pat. Appl., 50 pp.
CODEN: EPXXDW
DT Patent
LA English
FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|---|
| PI | EP 248594 | A2 | 19871209 | EP 1987-304720 | 19870528 |
| | EP 248594 | A3 | 19881117 | | |
| | EP 248594 | B1 | 19931124 | | |
| | R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE | | | | |
| | | | | US 1986-867996 | 19860529 |
| | | | | US 1987-42661 | 19870429 |
| | US 4826868 | A | 19890502 | US 1987-42661 | 19870429 |
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| NO 8702228 | A | 19871130 | NO 1987-2228 | 19870527 |
| NO 172236 | B | 19930315 | | |
| NO 172236 | C | 19930623 | | |
| | | | US 1986-867996 | 19860529 |
| | | | US 1987-42661 | 19870429 |
| AU 8773608 | A1 | 19871210 | AU 1987-73608 | 19870527 |
| AU 596844 | B2 | 19900517 | | |
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| | | | US 1987-42661 | 19870429 |
| ZA 8703842 | A | 19890125 | ZA 1987-3842 | 19870527 |
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| CA 1337122 | A1 | 19950926 | CA 1987-538137 | 19870527 |
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| | | | US 1987-42661 | 19870429 |
| FI 8702379 | A | 19871130 | FI 1987-2379 | 19870528 |
| FI 94340 | B | 19950515 | | |
| FI 94340 | C | 19950825 | | |
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| | | | US 1987-42661 | 19870429 |
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| ES 2059377 | T3 | 19941116 | ES 1987-304720 | 19870528 |
| | | | US 1986-867996 | 19860529 |
| | | | US 1987-42661 | 19870429 |
| HU 68247 | A2 | 19950628 | HU 1987-2466 | 19870528 |
| | | | US 1986-867996 | 19860529 |
| | | | US 1987-42661 | 19870429 |
| CN 87103953 | A | 19871209 | CN 1987-103953 | 19870529 |
| CN 1028227 | B | 19950419 | | |
| | | | US 1986-867996 | 19860529 |
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| JP 63022080 | A2 | 19880129 | JP 1987-134789 | 19870529 |
| JP 2512751 | B2 | 19960703 | | |
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| US 5164381 | A | 19921117 | US 1991-730515 | 19910712 |
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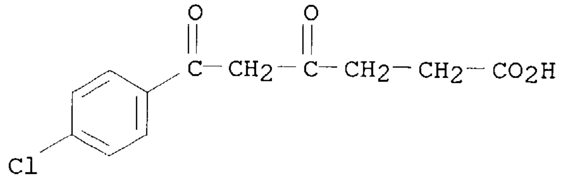
| | | | US 1987-42661 | 19870429 |
| | | | US 1989-339272 | 19890414 |

OS CASREACT 108:186735

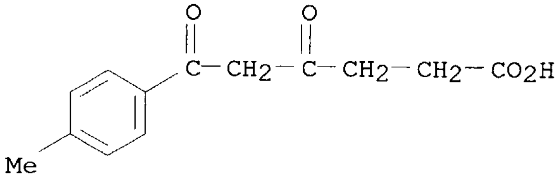
IT **111881-78-8P 114150-50-4P 114150-51-5P**
**114150-52-6P 114150-53-7P 114150-54-8P**
**114150-55-9P 114150-56-0P 114150-57-1P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, as antiinflammatory)

RN 111881-78-8 CAPLUS

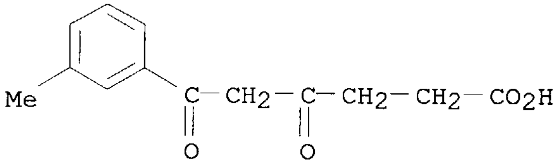
CN Benzenehexanoic acid, 4-chloro-$\gamma$,$\varepsilon$-dioxo- (9CI) (CA INDEX NAME)



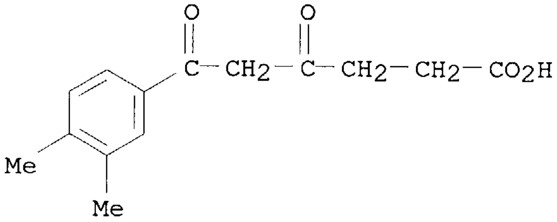
RN 114150-50-4 CAPLUS
CN Benzenehexanoic acid, 4-methyl-γ,ε-dioxo- (9CI) (CA INDEX NAME)



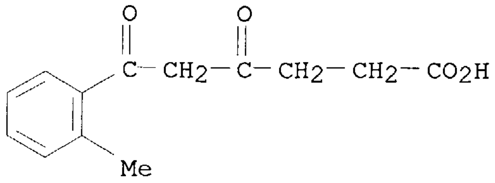
RN 114150-51-5 CAPLUS
CN Benzenehexanoic acid, 3-methyl-γ,ε-dioxo- (9CI) (CA INDEX NAME)



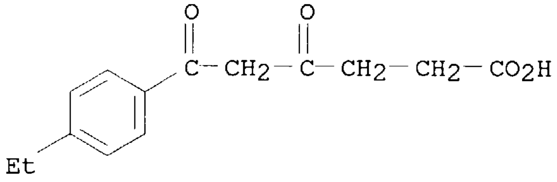
RN 114150-52-6 CAPLUS
CN Benzenehexanoic acid, 3,4-dimethyl-γ,ε-dioxo- (9CI) (CA INDEX NAME)



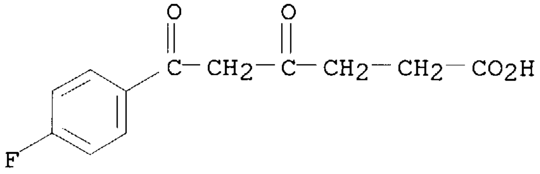
RN 114150-53-7 CAPLUS
CN Benzenehexanoic acid, 2-methyl-γ,ε-dioxo- (9CI) (CA INDEX NAME)



RN 114150-54-8 CAPLUS
CN Benzenehexanoic acid, 4-ethyl-γ,ε-dioxo- (9CI) (CA INDEX NAME)



RN 114150-55-9 CAPLUS
CN Benzenehexanoic acid, 4-fluoro-γ,ε-dioxo- (9CI) (CA INDEX NAME)



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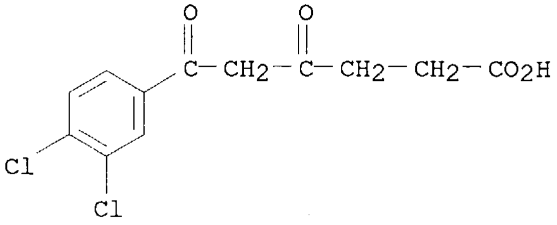
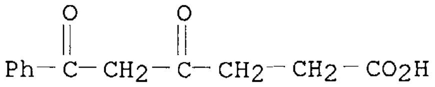


RN 114150-57-1 CAPLUS
CN Benzenehexanoic acid, γ,ε-dioxo- (9CI) (CA INDEX NAME)



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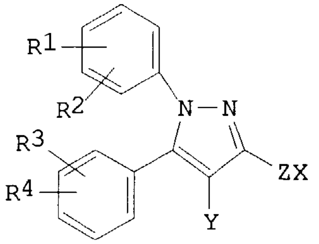
GI



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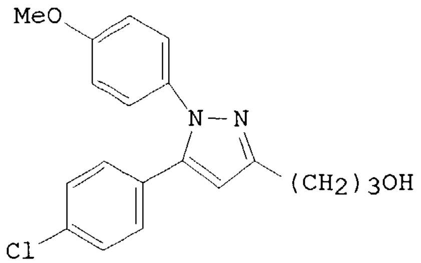

II

AB The title compds. [I; R1-R4 = H, alkoxy, Ph, halo, OH, alkylthio, alkylsulfonyl, NO2, CF3, amino, AcNH, CO2H, (un)substituted alkyl; R1R2, R3R4 = atoms to complete an (un)substituted benzo ring; X = (esterified) OH or CO2H, alkoxy, alkanoyl, acyl, amino, oximino, etc.; Y = H, alkyl, Br, Cl; Z = divalent, (un)substituted, (un)saturated C2-16 hydrocarbon residue] and their **pharmaceutically acceptable salts** were prepared as inflammation inhibitors. 4-ClC6H4COCH2CO(CH2)3OH was added to a mixture of 4-MeOC6H4NHNH2.HCl and pyridine in MeOH, and the resulting mixture stirred 1.5 h at room temperature to give 91% diphenylpyrazolepropanol II. In the rat paw edema test II had an ED50 of 3.6 mg/kg/day orally for 5 days.

L12 ANSWER 94 OF 100 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1987:156479 CAPLUS
DN 106:156479
TI Carbocyclic carboxamidines and related imidazoles and pyrimidines as adrenergic agents
IN Debernardis, John F.; Basha, Fatima Z.
PA Abbott Laboratories, USA
SO U.S., 15 pp. Cont.-in-part of U.S. Ser. No. 617,770, abandoned. CODEN: USXXAM
DT Patent
LA English
FAN.CNT 2

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|---|
| PI | US 4634705 | A | 19870106 | US 1986-838212 | 19860307 |
| | | | | US 1984-617770 | 19840606 |
| | CA 1259995 | A1 | 19890926 | CA 1985-483266 | 19850605 |
| | | | | US 1984-617770 | 19840606 |
| | JP 61007245 | A2 | 19860113 | JP 1985-121620 | 19850606 |
| | JP 06035444 | B4 | 19940511 | | |
| | | | | US 1984-617770 | 19840606 |

PATENT FAMILY INFORMATION:
FAN 1986:206777

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|---|
| PI | EP 166937 | A2 | 19860108 | EP 1985-106209 | 19850521 |
| | EP 166937 | A3 | 19860122 | | |
| | EP 166937 | B1 | 19910828 | | |

R: BE, CH, DE, FR, GB, IT, LI, NL, SE

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TERMINAL (ENTER 1, 2, 3, OR ?):2


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                  present
 NEWS  4  DEC 08  INPADOC: Legal Status data reloaded
 NEWS  5  SEP 29  DISSABS now available on STN
 NEWS  6  OCT 10  PCTFULL: Two new display fields added
 NEWS  7  OCT 21  BIOSIS file reloaded and enhanced
 NEWS  8  OCT 28  BIOSIS file segment of TOXCENTER reloaded and enhanced
 NEWS  9  NOV 24  MSDS-CCOHS file reloaded
 NEWS 10  DEC 08  CABA reloaded with left truncation
 NEWS 11  DEC 08  IMS file names changed
 NEWS 12  DEC 09  Experimental property data collected by CAS now available
                  in REGISTRY
 NEWS 13  DEC 09  STN Entry Date available for display in REGISTRY and CA/CAplus
 NEWS 14  DEC 17  DGENE: Two new display fields added
 NEWS 15  DEC 18  BIOTECHNO no longer updated
 NEWS 16  DEC 19  CROPU no longer updated; subscriber discount no longer
                  available
 NEWS 17  DEC 22  Additional INPI reactions and pre-1907 documents added to CAS
                  databases
 NEWS 18  DEC 22  IFIPAT/IFIUDB/IFICDB reloaded with new data and search fields
 NEWS 19  DEC 22  ABI-INFORM now available on STN
 NEWS 20  JAN 27  Source of Registration (SR) information in REGISTRY updated
                  and searchable
 NEWS 21  JAN 27  A new search aid, the Company Name Thesaurus, available in
                  CA/CAplus
 NEWS 22  FEB 05  German (DE) application and patent publication number format
                  changes
 NEWS 23  MAR 03  MEDLINE and LMEDLINE reloaded
 NEWS 24  MAR 03  MEDLINE file segment of TOXCENTER reloaded
 NEWS 25  MAR 03  FRANCEPAT now available on STN

 NEWS EXPRESS  MARCH 5 CURRENT WINDOWS VERSION IS V7.00A, CURRENT
               MACINTOSH VERSION IS V6.0b(ENG) AND V6.0Jb(JP),
               AND CURRENT DISCOVER FILE IS DATED 3 MARCH 2004
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specific topic.
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=> file reg
COST IN U.S. DOLLARS                               SINCE FILE      TOTAL
                                                        ENTRY    SESSION
FULL ESTIMATED COST                                      0.21       0.21

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DICTIONARY FILE UPDATES:   16 MAR 2004  HIGHEST RN 663883-43-0

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information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

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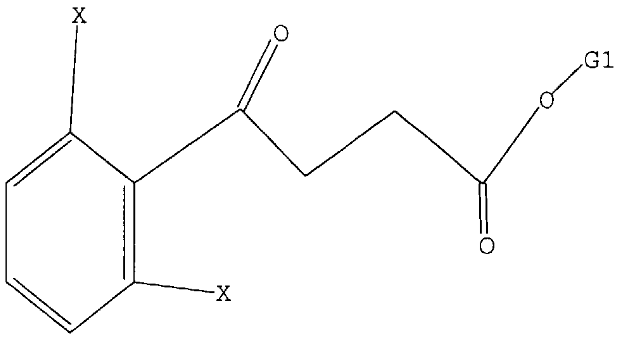

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G1 H,Ak


Structure attributes must be viewed using STN Express query preparation.


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FULL SCREEN SEARCH COMPLETED -    1744 TO ITERATE

100.0% PROCESSED    1744 ITERATIONS                           35 ANSWERS
SEARCH TIME: 00.00.04

L2           35 SEA SSS FUL L1

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COST IN U.S. DOLLARS                                SINCE FILE       TOTAL
                                                         ENTRY     SESSION
FULL ESTIMATED COST                                     155.42      155.63

FILE 'CAPLUS' ENTERED AT 11:26:36 ON 17 MAR 2004
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FILE COVERS 1907 - 17 Mar 2004  VOL 140 ISS 12
FILE LAST UPDATED: 16 Mar 2004  (20040316/ED)

  This file contains CAS Registry Numbers for easy and accurate
  substance identification.


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L3          24 L2
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L4             4 L2 AND SALT

=> s l2 and pharmaceutical
L5             1 L2 AND PHARMACEUTICAL

=> s l3 and pharmaceutical salts
L6             0 L3 AND PHARMACEUTICAL SALTS

=> s l3 and pharmaceutical salt
L7             0 L3 AND PHARMACEUTICAL SALT

=> d his

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L2             35 S L1 SSS FULL

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L5              1 S L2 AND PHARMACEUTICAL
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L7              0 S L3 AND PHARMACEUTICAL SALT

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L3   ANSWER 1 OF 24  CAPLUS  COPYRIGHT 2004 ACS on STN
AN   2003:603894  CAPLUS
DN   139:149330
TI   Preparation of 4-oxo-butenoic acids and related compounds for the
     treatment of breast cancer
IN   Miles, Howard; Yurjevich, Solodnikov Sergey; Petrovna, Krasnykh Olga;
     Valentinovna, Pimenova Elena; Goun, Elena A.
PA   University of Central Florida, USA
SO   U.S., 15 pp.
     CODEN: USXXAM
DT   Patent
LA   English
FAN.CNT 1
     PATENT NO.        KIND  DATE           APPLICATION NO.  DATE
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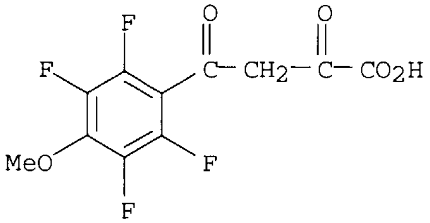
PI   US 6602907         B1   20030805       US 2002-164541   20020607
                                            US 2001-296823PP 20010608
     US 6686496         B1   20040203       US 2002-165027   20020607
                                            US 2001-296823PP 20010608
     US 6638975         B1   20031028       US 2002-309619   20021204
                                            US 2001-296823PP 20010608
                                            US 2002-164541 A320020607
     US 6703426         B1   20040309       US 2002-309536   20021204
                                            US 2001-296823PP 20010608
                                            US 2002-164541 A320020607
IT   572921-68-7P
     RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
```

(Uses)
(target compound; preparation of 4-oxo-butenoic acids and related compds. for
the treatment of breast cancer)

RN 572921-68-7 CAPLUS

CN Benzenebutanoic acid, 2,3,5,6-tetrafluoro-4-methoxy-α,γ-dioxo- (9CI) (CA INDEX NAME)



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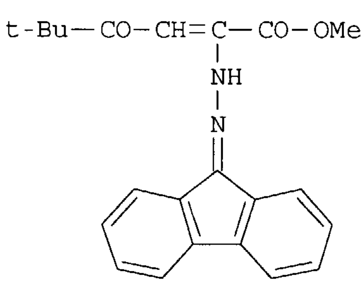

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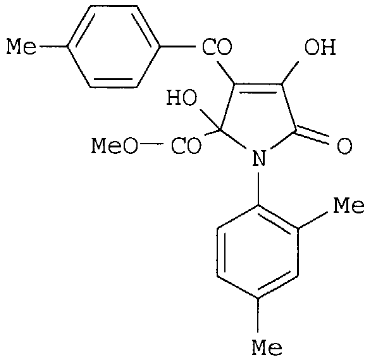

II

AB Title compds. I and II and related compds. are claimed useful for the treatment of breast carcinoma. For example, condensation of 2-hydroxy-5,5-dimethyl-4-oxohex-2-enoic acid Me ester and fluoren-9-ylidene hydrazine afforded claimed ester I in 68% yield. In human breast carcinoma cell growth inhibition and LD50 assays, 6-examples of 4-oxo-butenoic acids and related compds. exhibited 100% activity (sic) with LD50 values ranging from >200->3000 mg/kg., e.g., claimed ester I had 100% activity with LD50 value > 3000 mg/kg. Of note, 4-examples of 4-oxo-butenoic acids and related compds. posses at least "10 times lower acute toxicity compared to the most promising antitumor agent developed in the past three decades".

RE.CNT 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 2 OF 24 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2003:97391 CAPLUS
DN 138:137324
TI Preparation of phenylpropionic acid derivatives as α4 integrin inhibitors
IN Chiba, Akira; Sagi, Kazuyuki; Yoshimura, Toshihiko; Okuzumi, Tatsuya;

```
          or heteroaryl; E = CO, CHOH; G-G1 = CH-CH2, C:CH; J, J1 = H, halo, lower
          alkyl, lower alkoxy, NO2] are prepared  These derivs. exhibit α4
          integrin inhibiting activity and are useful as therapeutic or preventive
          agents for various diseases in which α4 integrin participates, e.g.,
          inflammatory diseases in which integrin-dependent adhesion participates.
          The above diseases include rheumatoid arthritis, inflammatory bowel
          diseases, systemic lupus erythematosus, multiple sclerosis, Sjoegren's
          syndrome, asthma, psoriasis, allergy, diabetes, cardiovascular diseases,
          arteriosclerosis, restenosis, tumor proliferation, tumor metastasis, and
          transplant rejection.  Thus, cyclization of 4-oxo-4-phenylbutanoic acid in
          Ac2O at 90° gave 43% 5-phenyl-2,3-dihydrofuran-2-one which
          underwent condensation with 4-nitrobenzaldehyde in the presence of NaOAc
          in Ac2O at 80° for 1 h to give 93% 3-(4-nitrobenzylidene)-5-phenyl-
          2,3-dihydrofuran-2-one (II).  Ring-opening methanolysis of II with NaOMe
          in MeOH gave 84% 2-(4-nitrobenzylidene)-4-oxo-4-phenylbutanoic acid Me
          ester which was hydrogenated over 7.5% Pd/C in ethanol to give 28%
          2-(4-aminobenzyl)-4-oxo-4-phenylbutanoic acid Me ester (III).
          Cyclocondensation of III with 2-isocyanatobenzoic acid Me ester in MeCN at
          70° for 2 h and then at 70° for 11 h in the presence of Et3N
          gave 80% 2-[4-(2,4-dioxo-1,2,3,4-tetrahydroquinazolin-3-yl)benzyl]-4-oxo-4-
          phenylbutanoic acid Me ester (IV; R = X = H, R24 = Me) which was
          methylated by MeI in the presence of K2CO3 in DMF for 1 h to quant. give
          IV (R = R24 = Me, X = H).  Saponification of the latter compound with aqueous
LiOH in
          aqueous MeOH followed by acidification with 1 N aqueous HCl gave 54% IV (R =
Me,
          R24 = X = H).  IV (R = Me, R24 = X = H) and IV (R = Me, R24 = H, X = Cl)
          in vitro inhibited the binding of vascular cellular adhesion mol.-1
          (VCAM-1) to human B cell lymphoma cell expressing integrin α4β7
          with IC50 of ≤20 to <100 μmol/L and ≤0.9 μmol/L, resp.
RE.CNT  12      THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD
                ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3        ANSWER 3 OF 24  CAPLUS  COPYRIGHT 2004 ACS on STN
AN        2002:964135  CAPLUS
DN        138:24543
TI        Preparation of benzyloxyphenyloxobutyrates and related compounds for the
          treatment of metabolic disorders
IN        Sharma, Shalini; Von Borstel, Reid W.; Hodge, Kirvin L.
PA        Wellstat Therapeutics Corporation, USA
SO        PCT Int. Appl., 242 pp.
          CODEN: PIXXD2
DT        Patent
LA        English
FAN.CNT 1
          PATENT NO.          KIND  DATE            APPLICATION NO.   DATE
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PI        WO 2002100341        A2   20021219        WO 2002-US18388   20020612
              W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
                  CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
                  GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
                  LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
                  PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ,
                  UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU,
                  TJ, TM
              RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH,
                  CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR,
                  BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
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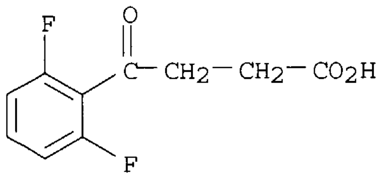
US 2001-297282PP 20010612
US 2003149107 A1 20030807 US 2002-167839 20020612
US 2001-297282PP 20010612

OS MARPAT 138:24543

IT **478162-62-8P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of benzyloxyphenyloxobutyrates and related compds. for treatment of metabolic disorders)

RN 478162-62-8 CAPLUS

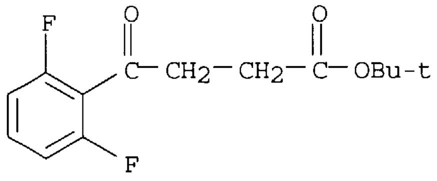
CN Benzenebutanoic acid, 2,6-difluoro-γ-oxo- (9CI) (CA INDEX NAME)



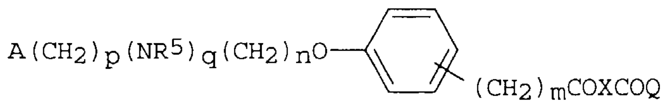
IT **478163-14-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of benzyloxyphenyloxobutyrates and related compds. for treatment of metabolic disorders)

RN 478163-14-3 CAPLUS

CN Benzenebutanoic acid, 2,6-difluoro-γ-oxo-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



GI



I

AB Biol. active title compds. [I; n = 1, 2; m, q, p = 0, 1; R5 = alkyl; R9 = H, halo, alkoxy; A = (halo-, alkyl-, perfluoromethyl-, alkoxy-, perfluoromethoxy-substituted) Ph, (Me-, Et-substituted) cycloalkyl, 5-6 membered heteroarom. ring having 1-2 N, S, O atoms; X = CH2, Q = OR1, R1 = Et; or X = CH2CR12R13, CH2CH(NHAc), Q = OR1, R1 = H, alkyl; or X = CH2CH2, Q = NR10R11; R12, R13 = H, Me; 1 of R10, R11 = H, alkyl, OH, the other = H, alkyl], were prepared Thus, 4-(2-fluorobenzyloxy)acetophenone (preparation given) in THF and DMPU was treated with a solution of Li

Izawa, Hiroyuki; Murata, Masahiro
PA Ajinomoto Co., Inc., Japan
SO PCT Int. Appl., 57 pp.
CODEN: PIXXD2
DT Patent
LA Japanese
FAN.CNT 1

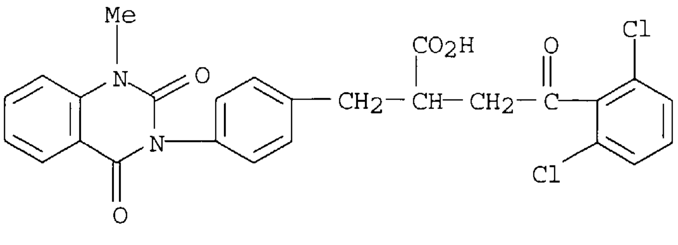
| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|---|
| PI | WO 2003010135 | A1 | 20030206 | WO 2002-JP7543 | 20020725 |

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

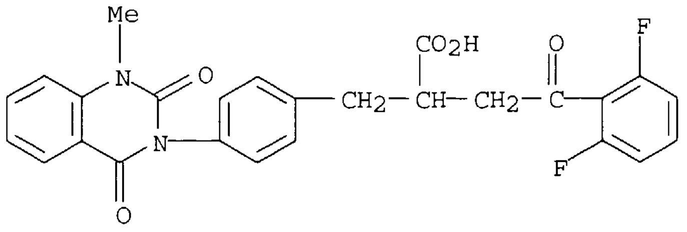
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

JP 2001-225749 A 20010726

OS MARPAT 138:137324
IT **493004-40-3P**, 4-(2,6-Dichlorophenyl)-2-[4-(1-methyl-2,4-dioxo-1,2,3,4-tetrahydroquinazolin-3-yl)benzyl]-4-oxobutanoic acid **493004-41-4P**, 4-(2,6-Difluorophenyl)-2-[4-(1-methyl-2,4-dioxo-1,2,3,4-tetrahydroquinazolin-3-yl)benzyl]-4-oxobutanoic acid **493004-43-6P**, (E)-2-[2-(2,6-Dichlorophenyl)-2-oxoethyl]-3-[4-(1-methyl-2,4-dioxo-1,2,3,4-tetrahydroquinazolin-3-yl)phenyl]-2-propenoic acid **493004-44-7P**, 4-(2,6-Dichlorophenyl)-2-[4-[[[(2-methoxycarbonylphenyl)amino]carbonyl]amino]benzyl]-4-oxobutanoic acid
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of phenylpropionic acid derivs. as α4 integrin inhibitors for prevention or treatment of α4 integrin-participating various diseases)
RN 493004-40-3 CAPLUS
CN Benzenebutanoic acid, 2,6-dichloro-α-[[4-(1,4-dihydro-1-methyl-2,4-dioxo-3(2H)-quinazolinyl)phenyl]methyl]-γ-oxo- (9CI) (CA INDEX NAME)

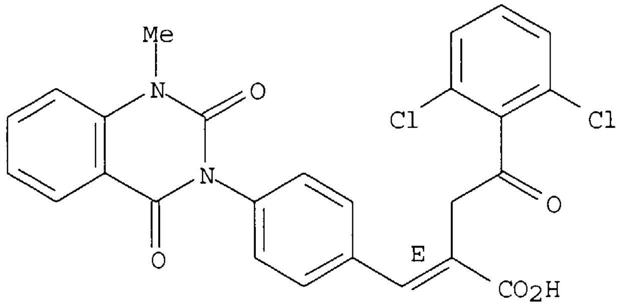


RN 493004-41-4 CAPLUS
CN Benzenebutanoic acid, α-[[4-(1,4-dihydro-1-methyl-2,4-dioxo-3(2H)-quinazolinyl)phenyl]methyl]-2,6-difluoro-γ-oxo- (9CI) (CA INDEX NAME)

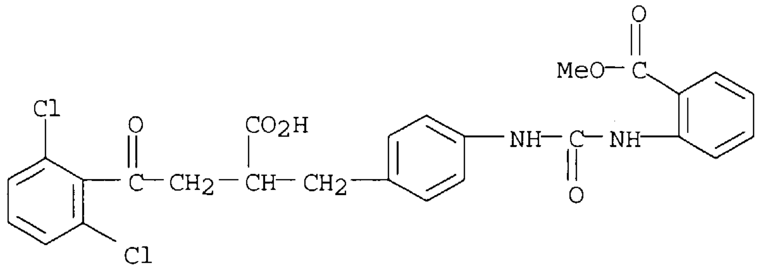


RN 493004-43-6 CAPLUS
CN Benzenebutanoic acid, 2,6-dichloro-α-[[4-(1,4-dihydro-1-methyl-2,4-dioxo-3(2H)-quinazolinyl)phenyl]methylene]-γ-oxo-, (αE)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 493004-44-7 CAPLUS
CN Benzenebutanoic acid, 2,6-dichloro-α-[[4-[[[[2-(methoxycarbonyl)phenyl]amino]carbonyl]amino]phenyl]methyl]-γ-oxo- (9CI) (CA INDEX NAME)

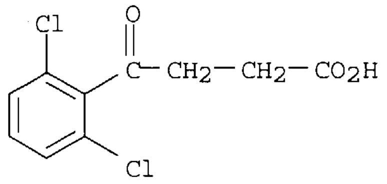


IT **493004-51-6P**, 4-(2,6-Dichlorophenyl)-4-oxobutanoic acid **493004-53-8P**, 4-(2,6-Difluorophenyl)-4-oxobutanoic acid ethyl ester **493004-54-9P**, (E)-2-[2-(2,6-Dichlorophenyl)-2-oxoethyl]-3-(4-nitrophenyl)-2-propenoic acid methyl ester **493004-55-0P**, (E)-2-[2-(2,6-Dichlorophenyl)-2-oxoethyl]-3-(4-aminophenyl)-2-propenoic acid methyl ester **493004-57-2P**, 4-(2,6-Dichlorophenyl)-2-[4-(1-methyl-2,4-dioxo-1,2,3,4-tetrahydroquinazolin-3-yl)benzyl]-4-oxobutanoic acid methyl ester
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of phenylpropionic acid derivs. as α4 integrin inhibitors for prevention or treatment of α4 integrin-participating various diseases)

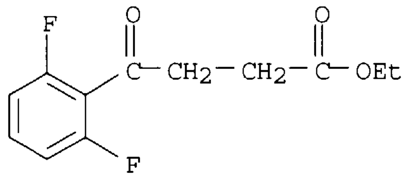
RN 493004-51-6 CAPLUS

CN Benzenebutanoic acid, 2,6-dichloro-γ-oxo- (9CI) (CA INDEX NAME)



RN 493004-53-8 CAPLUS

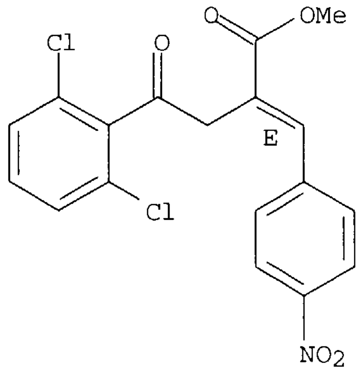
CN Benzenebutanoic acid, 2,6-difluoro-γ-oxo-, ethyl ester (9CI) (CA INDEX NAME)



RN 493004-54-9 CAPLUS

CN Benzenebutanoic acid, 2,6-dichloro-α-[(4-nitrophenyl)methylene]-γ-oxo-, methyl ester, (αE)- (9CI) (CA INDEX NAME)

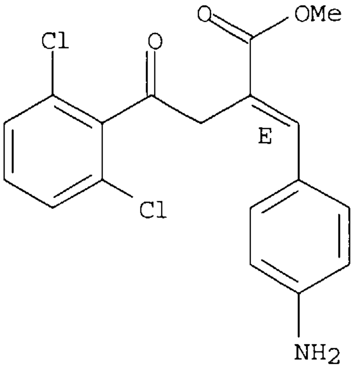
Double bond geometry as shown.



RN 493004-55-0 CAPLUS

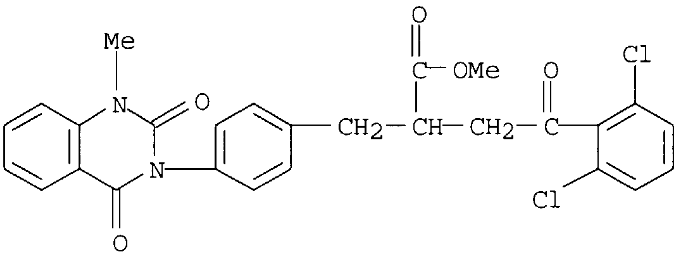
CN Benzenebutanoic acid, α-[(4-aminophenyl)methylene]-2,6-dichloro-γ-oxo-, methyl ester, (αE)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 493004-57-2 CAPLUS

CN Benzenebutanoic acid, 2,6-dichloro-α-[[4-(1,4-dihydro-1-methyl-2,4-dioxo-3(2H)-quinazolinyl)phenyl]methyl]-γ-oxo-, methyl ester (9CI) (CA INDEX NAME)



GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Phenylpropionic acid derivs. represented by the general formula (I) [wherein A = Q-Q4, (un)substituted Ph, NR1-Z, NR1-CO-Z, NR1-SO2-Z, NR1-CONH-Z, NR1-C(:S)-NH-Z; wherein Z = (un)substituted Ph, lower alkyl, lower alkenyl, lower alkynyl, cycloalkyl, cycloalkyl-lower alkyl, cycloalkyl-lower alkenyl, or cycloalkyl-lower alkynyl optionally containing a heteroatoms in the cycloalkyl ring, aryl, heteroaryl, cycloalkyl, etc.; R10-R17, R21, R22, R24, R25 = H, halo, OH, lower alkyl, lower alkenyl, lower alkynyl, cycloalkyl, cycloalkyl-lower alkyl, cycloalkyl-lower alkenyl, or cycloalkyl-lower alkynyl optionally containing a heteroatoms in the cycloalkyl ring, aryl, heteroaryl, aryl-lower alkyl, heteroaryl-lower alkyl, lower alkoxy, etc.; the ring Arm = benzene ring, cycloalkyl or aromatic ring containing 0, 1, 2,3, or 4 heteroatom(s) selected from O, S, and N;

R9, R20, R23 = O, (un)substituted NH, S; R18, R19 = H, lower alkyl, lower alkenyl, lower alkynyl, aryl, heteroaryl, aryl-lower alkyl, cycloalkyl, cycloalkyl-lower alkyl, cycloalkyl-lower alkenyl, or cycloalkyl-lower alkynyl optionally containing a heteroatoms in the cycloalkyl ring, etc.; B = HO, alkoxy, hydroxyl NH2, lower alkylamino; D = each (un)substituted lower alkyl, cycloalkylaryl optionally containing a heteroatoms in the ring, aryl,

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L3   ANSWER 16 OF 24  CAPLUS  COPYRIGHT 2004 ACS on STN
AN   1995:932936  CAPLUS
DN   124:117239
TI   Reaction of copper chelates of (polyfluoroacyl)pyruvic acid esters with
     hydrazine and o-phenylenediamine
AU   Saloutin, V. I.; Skryabina, Z. E.; Kondrat'ev, P. N.; Perevalov, S. G.
CS   Inst. Org. Sint., Ural. Otd. RAN, Yekaterinburg, Russia
SO   Zhurnal Organicheskoi Khimii (1995), 31(2), 266-9
     CODEN: ZORKAE; ISSN: 0514-7492
PB   Nauka
DT   Journal
LA   Russian
IT   161037-54-3, Ethyl (pentafluorobenzoyl)pyruvate
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (cyclocondensation with hydrazine and phenylenediamine)
RN   161037-54-3  CAPLUS
CN   Benzenebutanoic acid, 2,3,4,5,6-pentafluoro-α,γ-dioxo-, ethyl
     ester (9CI)  (CA INDEX NAME)
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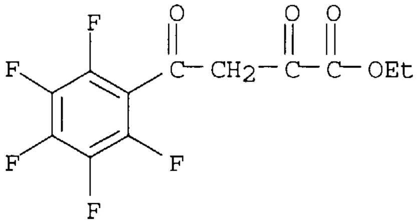

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AB   Polyfluorinated derivs. of pyrazolecarboxylates and quinoxalinones were
     prepared by the title reactions.

L3   ANSWER 17 OF 24  CAPLUS  COPYRIGHT 2004 ACS on STN
AN   1995:896100  CAPLUS
DN   123:313934
TI   Preparation of 2(5H)-furanones, 2(5H)-thiophenones, 2(5H)-pyrrolones and
     benzodioxolyls as endothelin antagonists
IN   Berryman, Kent Alan; Doherty, Annette Marian; Edmunds, Jeremy John; Patt,
     William Chester; Plummer, Mark Stephen; Repine, Joseph Thomas
PA   Warner-Lambert Co., USA
SO   PCT Int. Appl., 423 pp.
     CODEN: PIXXD2
DT   Patent
LA   English
FAN.CNT 2
     PATENT NO.        KIND  DATE          APPLICATION NO.  DATE
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PI   WO 9505376         A1   19950223      WO 1994-US9091   19940809
         W:  AU, CA, CZ, FI, HU, JP, KR, NO, NZ, RU, SK
         RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE
                                           US 1993-109751   19930819
                                           US 1994-217578   19940324
                                           US 1994-278882   19940726
     CA 2165567         AA   19950223      CA 1994-2165567  19940809
                                           US 1993-109751   19930819
                                           US 1994-217578   19940324
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                                                US 1994-278882   19940726
     AU 9475617        A1   19950314            AU 1994-75617    19940809
     AU 693110         B2   19980625
                                                US 1993-109751   19930819
                                                US 1994-217578   19940324
                                                US 1994-278882   19940726
                                                WO 1994-US9091   19940809
     EP 714391         A1   19960605            EP 1994-925831   19940809
         R:  AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE
                                                US 1993-109751   19930819
                                                US 1994-217578   19940324
                                                US 1994-278882   19940726
                                                WO 1994-US9091   19940809
     HU 74179          A2   19961128            HU 1996-365      19940809
                                                US 1993-109751   19930819
                                                US 1994-217578   19940324
                                                US 1994-278882   19940726
     JP 09501920       T2   19970225            JP 1994-507074   19940809
                                                US 1993-109751   19930819
                                                US 1994-217578   19940324
                                                US 1994-278882   19940726
                                                WO 1994-US9091   19940809
     ZA 9406265        A    19960219            ZA 1994-6265     19940818
                                                US 1993-109751   19930819
     FI 9600671        A    19960419            FI 1996-671      19960214
                                                US 1993-109751   19930819
                                                US 1994-217578   19940324
                                                US 1994-278882   19940726
                                                WO 1994-US9091   19940809
     NO 9600629        A    19960216            NO 1996-629      19960216
                                                US 1993-109751   19930819
                                                US 1994-217578   19940324
                                                US 1994-278882   19940726
                                                WO 1994-US9091   19940809
PATENT FAMILY INFORMATION:
FAN  1997:780649
     PATENT NO.        KIND  DATE               APPLICATION NO.  DATE
     ---------------   ----  --------           ---------------  --------
PI   US 5691373         A    19971125           US 1995-384083   19950206
                                                US 1993-109751   19930819
                                                US 1994-217578   19940324
                                                US 1994-278882   19940726
     CA 2165567         AA   19950223           CA 1994-2165567  19940809
                                                US 1993-109751   19930819
                                                US 1994-217578   19940324
                                                US 1994-278882   19940726
     HU 74179           A2   19961128           HU 1996-365      19940809
                                                US 1993-109751   19930819
                                                US 1994-217578   19940324
                                                US 1994-278882   19940726
     ZA 9406265         A    19960219           ZA 1994-6265     19940818
                                                US 1993-109751   19930819
     US 6017916         A    20000125           US 1997-787423   19970122
                                                US 1993-109751   19930819
                                                US 1994-217578   19940324
                                                US 1994-278882   19940726
                                                US 1995-384083   19950206
OS   MARPAT 123:313934
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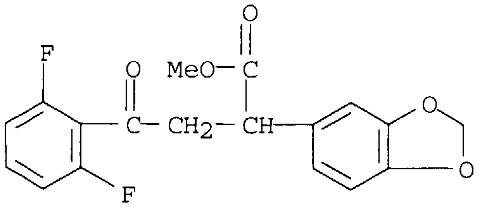
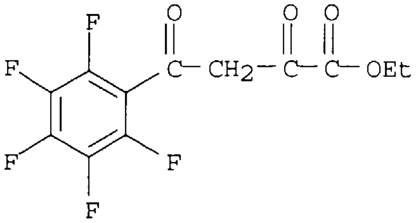
IT **169803-96-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 2(5H)-furanones, 2(5H)-thiophenones, 2(5H)-pyrrolones and benzodioxolyls as endothelin antagonists)
RN 169803-96-7 CAPLUS
CN 1,3-Benzodioxole-5-acetic acid, α-[2-(2,6-difluorophenyl)-2-oxoethyl]-, methyl ester (9CI) (CA INDEX NAME)



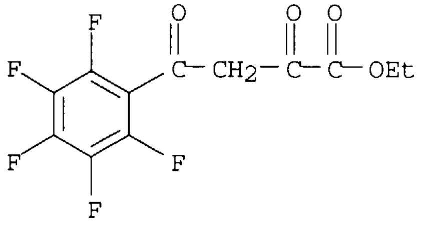
AB Title compds. and salts thereof are prepared Chalcones were treated with KCN to give nitrile addition products, hydrolysis of which gave the corresponding acids which were then cyclized with aldehydes give 2(5H)-furanones. In vitro and in vivo antagonism was demonstrated. Title compds. are claimed for many human diseases in which endothelin is involved.

L3 ANSWER 18 OF 24 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1995:846347 CAPLUS
DN 124:55777
TI Synthesis of 2(3)-(ethoxycarbonyl)-5,6,7,8-tetrafluorochromones
AU Saloutin, V. I.; Skryabina, Z. E.; Bazyl, I. T.; Chupakhin, O. N.
CS Inst. Org. Chem., Ural Br. Russ. Acad. Sci., Yekaterinburg, 620219, Russia
SO Izvestiya Akademii Nauk, Seriya Khimicheskaya (1993), (2), 362-4
CODEN: IASKEA
PB Nauka
DT Journal
LA Russian
OS CASREACT 124:55777
IT **161037-54-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(for preparation of (ethoxycarbonyl)tetrafluorochromes)
RN 161037-54-3 CAPLUS
CN Benzenebutanoic acid, 2,3,4,5,6-pentafluoro-α,γ-dioxo-, ethyl ester (9CI) (CA INDEX NAME)

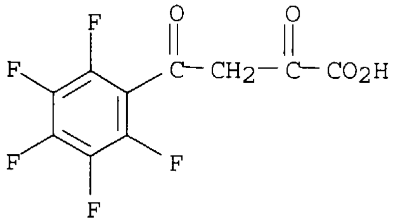


AB The hitherto unknown Et pentafluorobenzoylpyruvate was prepared by condensing pentafluoroacetophenone with di-Et oxalate. Intramol. cyclization of this ester or its Cu(II), and of Et 2-ethoxymethylenepentafluorobenzoylacetate affords novel 2- and 3-ethoxycarbonyl-5,6,7,8-tetrafluorochromones. Hydrolysis of the latter followed by decarboxylation gives 5,6,7,8-tetrafluorochrome.

L3 ANSWER 19 OF 24 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1995:541990 CAPLUS
DN 123:198592
TI Reaction of (pentafluorobenzoyl)pyruvic acid with amines
AU Saloutin, V. I.; Bazyl', I. T.; Skryabina, Z. E.; Kondrat'ev, P. N.; Chupakhin, O. N.
CS Inst. Org. Synth., Ural Branch Russian Acad. Sci., Ekaterinburg, 620219, Russia
SO Izvestiya Akademii Nauk, Seriya Khimicheskaya (1994), (2), 299-302
CODEN: IASKEA
PB Institut Organicheskoi Khimii im. N. D. Zelinskogo Rossiiskoi Akademii Nauk
DT Journal
LA Russian
IT **161037-54-3**, Ethyl (pentafluorobenzoyl)pyruvate
RL: RCT (Reactant); RACT (Reactant or reagent)
(hydrolysis of)
RN 161037-54-3 CAPLUS
CN Benzenebutanoic acid, 2,3,4,5,6-pentafluoro-α,γ-dioxo-, ethyl ester (9CI) (CA INDEX NAME)



IT **162188-41-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(reaction of (pentafluorobenzoyl)pyruvic acid with amines)
RN 162188-41-2 CAPLUS
CN Benzenebutanoic acid, 2,3,4,5,6-pentafluoro-α,γ-dioxo- (9CI) (CA INDEX NAME)



AB The title reactions give enamines and then N-substituted

1,4-dihydro-4-oxoquinoline-2-carboxylic acids by intramol. cyclization. Ammonia and triethylamine favor cyclization of (pentafluorobenzoyl)pyruvic acid to 2-carboxychromone.

L3 ANSWER 20 OF 24 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1995:295954 CAPLUS

DN 122:132911

TI Reaction of 2-ethoxycarbonyl(carboxy)-5,6,7,8-tetrafluorochromones with N-nucleophiles

AU Saloutin, V. I.; Bazyl, I. T.; Skryabina, Z. E.; Chupakhin, O. N.

CS Inst. Org. Synthesis, Ural Branch Russian Academy Sciences, Ekaterinburg, 620219, Russia

SO Izvestiya Akademii Nauk, Seriya Khimicheskaya (1994), (5), 904-7
CODEN: IASKEA

PB Institut Organicheskoi Khimii im. N. D. Zelinskogo Rossiiskoi Akademii Nauk

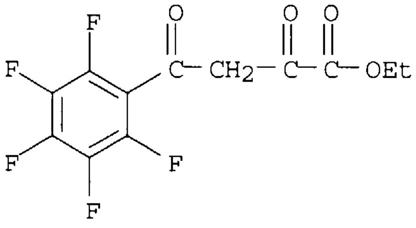
DT Journal

LA Russian

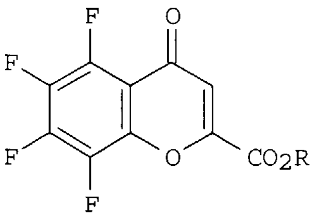
IT **161037-54-3**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction with amines)

RN 161037-54-3 CAPLUS

CN Benzenebutanoic acid, 2,3,4,5,6-pentafluoro-α,γ-dioxo-, ethyl ester (9CI) (CA INDEX NAME)



GI



I

AB The direction of reactions of title compds. (I; R = Et, H) with ammonia, methylamine, hexylamine, and aniline depends on the inductive effect of CO2R and on the basicity of the amine. Nucleophilic aromatic replacement of fluorine takes place in the reaction of I (R = Et) with secondary amines (morpholine, N-methylpiperazine) and ethylenediamine.

L3 ANSWER 21 OF 24 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1995:142394 CAPLUS